Single-photon scattering on a strongly dressed atom

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We develop the generalized rotating-wave approximation (GRWA) approach (Phys. Rev. Lett. **99**, 173601 (2007)) to study the single-photon scattering on a two-level system (TLS) with arbitrarily strong coupling to a local mode in a one-dimensional (1D) coupled resonator array. We calculate the scattering amplitudes analytically, and the independent numerical results show that our approach works well in a broad parameter region. Especially, when the resonator mode is far-off resonance with the TLS, we obtain more reasonable results than the ones from the standard adiabatic approximation. Our approach is further extended to the cases with a 1D resonator array strongly coupled to more than one TLSs.

I. INTRODUCTION

Recently, many attentions have been paid to the photon transport in a low-dimensional array of coupled resonators [1–25] or a one-dimensional (1D) wave guide [24–49], which plays crucial roles in the realization of all-optical quantum devices. In these systems, the two-level or multi-level devices coupled to the resonators or wave guides can be used as quantum switches to control the scattering or transport of the photons.

Up to now, the single-photon scattering amplitudes in the 1D resonator arrays or wave guides coupled to a single two-level system (TLS) [1–6, 25, 28–33] or a single three-level system [15, 41, 47, 48] or multi quantum devices [8–12, 34–38] have been well-investigated by different authors.The relevant multi-photon scattering amplitudes [21–27, 42–46] are also studied. To our knowledge, all these studies are based on the rotating-wave approximation which is applicable under the conditions that the frequencies of the two-level or multi-level system are very close to the photon frequencies in the resonators or wave guides, and the intensities of the coupling between the two-level or multi-level system and the photons are much smaller than their frequencies, namely, in the weak-coupling limit.

In the experiments, the 1D resonator arrays or wave guides can be realized with photonic crystals [50, 51], superconducting transmission line resonators [12–14, 29, 47, 52] or other solid devices, while the two-level or multi-level systems can be implemented with either natural atoms or the solid-state artificial atoms. In the hybrid systems of solid-state devices, it has been predicted that [53–56] one can realize ultra-strong TLS-photon coupling with intensities comparable or even higher than the photon frequencies. On the other hand, the frequency of the solid-state TLS can also be controlled easily in a

broad region. Therefore, in the quantum network based on solid-state devices it is possible to reach the strong-coupling and far-off resonance regime where the conditions of rotating-wave approximation are violated. In these parameter regions, we need to develop new methods for the scattering between the flying photon and the TLS, and then investigate the possible new effects given by the strong TLS-photon coupling to the photonic transport.

In this paper, we study the single photon scattering on the TLS, which strongly couples to the local mode of the resonators. Beyond the rotating-wave approximation, we develop an analytical approach for the approximate calculation of the single-photon scattering amplitudes in a 1D single-mode-resonator array coupled to a single TLS. Our method is based on the generalized rotating-wave approximation (GRWA) [57] developed by Irish for the system with a single TLS coupled to a single-mode bosonic field.

With our GRWA approach we obtain the single-photon scattering amplitudes under the condition that the photon hopping between different resonators is weak enough. We will show that our approach works significantly well in a very broad parameter region, including the region where the rotating-wave approximation is applicable and the one where the TLS-photon coupling is strong while the frequency of the TLS is close to or smaller than the photon frequency.

Especially, in the far-off resonance region where the TLS frequency is much smaller than the flying photon, the standard adiabatic approximation does not work well in the current hybrid system, while our approach still provides good results. On the other hand, when photon-TLS coupling is strong enough, our GRWA approach shows that the single-photon scattering by the TLS becomes equivalent to the transport of a single photon in a 1D resonator array in which the frequency of a certain resonator is shifted. Then our results are furthermore simplified and one can make reasonable qualitative estimations for the photon transport characters, even without

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the quantitative calculations. We also show that, our GRWA approach can be generalized to the systems with a 1D single-mode-resonator array coupled with more than one TLS.

This paper is organized as follows: In Sec. II, we develop the GRWA approach for the hybrid system of a 1D resonator array coupled to a single TLS. In Sec. III, we analytically calculate the single-photon scattering amplitudes in such a system with our GRWA approach and compare our results with the numerical results. In Sec. IV, we discuss the single-photon scattering problem in the cases of strong TLS-photon coupling. In Sec. V, we show the GRWA approach in the system with more than one TLS. There are several discussions and conclusions in Sec. VI.

II. THE GRWA FOR THE TLS-COUPLED 1D RESONATOR ARRAY

In this paper we consider the transmission of a single photon in a 1D single-mode-resonator array coupled to a TLS which is located in a specific resonator. To obtain the reasonable analytical results beyond the rotating-wave approximation, in this section we will generalize the GRWA approach proposed by Irish in Ref. [57] for a single resonator coupled to a TLS to our current hybrid system of resonator array. We will first show the adiabatic approximation in our system for the cases where the frequency of the TLS is much smaller than the photon frequency, and then develop the GRWA approach as an improvement of the adiabatic approximation. For the reader's convenience, in appendix A we introduce Irish's GRWA approach for the system with a single resonator in the view of adiabatic approximation.

A. The system and Hamiltonian

As shown in Fig. 1, we consider a 1D array of infinite identical single-mode resonators with a TLS located inside a certain resonator, which is marked as the 0-th resonator in the array. We further assume that the photons can hop between neighbor resonators. Then the total system is modeled by the Hamiltonian $H = H_C + H_A + H_I$, where the tight-binding Hamiltonian H_C of the resonator array is

$$H_C = \omega \sum_{j=-\infty}^{+\infty} a_j^\dagger a_j - \xi \sum_{j=-\infty}^{+\infty} (a_j^\dagger a_{j+1} + h.c.). \quad (1)$$

Here ω is the frequency of the photons in the resonators, ξ is the hopping intensity or the inter-resonator coupling strength, a_j and $a_j^\dagger$ are the annihilation and creation operators of the photons in the j-th resonator respectively.

In this paper we assume the weak-hopping condition
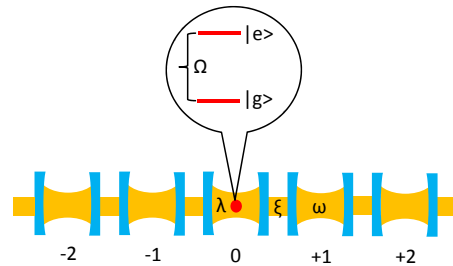
$$|\xi| << \omega \quad (2)$$

FIG. 1: (Color online) Schematic configuration for the hybrid system of a 1D resonator array interacting with a TLS. The frequency of the photon in each resonator is ω, while the intensity of the photonic hopping is ξ. The TLS with frequency Ω is localized at the 0-th resonator and coupled to the photon with coupling strength λ.

is satisfied. Therefore the term $a_j^\dagger a_{j+1}^\dagger + h.c.$ has been neglected in our consideration. This condition also provides us a small parameter ξ/ω which is very useful in the following calculation.

The Hamiltonian H_A of the TLS and the interaction H_I between the TLS and the photons in the 0-th resonator are

$$H_A = \frac{\Omega}{2}\sigma_z \quad (3)$$

and

$$H_I = \lambda\sigma_x(a_0^\dagger + a_0) \quad (4)$$

respectively. Here Ω is the energy spacing between the ground state $|g\rangle$ and the excited state $|e\rangle$ of the TLS, λ is the coupling intensity and the Pauli operators σ_z and σ_x are defined as $\sigma_z = |e\rangle\langle e| - |g\rangle\langle g|$ and $\sigma_x = |e\rangle\langle g| + |g\rangle\langle e|$.

B. The adiabatic approximation for the TLS-coupled 1D resonator array

In this and the next subsections, we develop the GRWA approach for the TLS-coupled 1D resonator array. To this end, in this section we first formally develop the adiabatic approximation for our system in the far-off resonance region with $\Omega << \omega$. We will show that, due to the energy band structure of the photons, the adiabatic approximation *cannot* be used in our hybrid system, even in the far-off resonance case. However, as shown in the next subsection, we can also develop the GRWA approach as an improvement of this formal adiabatic approach, and the intrinsic problem of the adiabatic approximation in our system is naturally overcome by our GRWA approach. Finally, our approach is applicable in a broad parameter region, including the cases of $\Omega << \omega$ and $\Omega \sim \omega$.

Under the far-off resonance condition $\Omega << \omega$, the TLS is considered to be the slowly-varying part of the system, while the 1D resonator-array is the fast-varying

one. Then we decompose the total Hamiltonian H as $H = H_1 + H_2$ where $H_1 = H_C + H_I$ is the Hamiltonian of the fast-varying part together with the interaction and $H_2 = H_A$ is the Hamiltonian of the slow-varying TLS.

The straightforward calculation shows that H_1 has the eigen-states

$$|\pm, \vec{n}\rangle = U \prod_k \frac{1}{\sqrt{n(k)!}} A(k)^{\dagger n(k)} |0\rangle \otimes |\pm\rangle. \qquad (5)$$

Here the TLS states $|\pm\rangle$ are the eigen-states of the operator σ_x with eigen-values ± 1, and $|0\rangle$ is the vacuum state of the resonator array. The photon momentum k can take any value in the region $(-\pi, \pi]$, the creation operator $A(k)^{\dagger}$ for a photon with momentum k is given by

$$A(k)^{\dagger} = \frac{1}{\sqrt{2\pi}} \sum_{l=-\infty}^{+\infty} e^{ikl} a_l^{\dagger}, \qquad (6)$$

and

$$\vec{n} = (n(k_1), n(k_2), ...) \qquad (7)$$

is the set of all the numbers $n(k)$.

The operator U in Eq. (5) is determined by

$$U^{-1} H_1 U = \omega \sum_{j=-\infty}^{+\infty} a_j^{\dagger} a_j - \xi \sum_{j=-\infty}^{+\infty} (a_j^{\dagger} a_{j+1} + h.c.) - \mathcal{C}, \qquad (8)$$

with $\mathcal{C}$ an unimportant c-number. This equation leads to the result

$$U = \prod_{j=-\infty}^{+\infty} \exp[\alpha_j \sigma_x (a_j^{\dagger} - a_j)] \qquad (9)$$

with

$$\alpha_j = \frac{\lambda \omega_1}{2\xi^2 - \omega \omega_1} \left(\frac{\xi}{\omega_1} \right)^{|j|}, \qquad (10)$$

where

$$\omega_1 = (\omega + \sqrt{\omega^2 - 4\xi^2})/2. \qquad (11)$$

The results in Eqs.(10,11) are derived in appendix B. It is pointed out that the parameter α_j exponentially decays to zero in the limit $|j| \to \infty$.

Obviously, the eigen-energy of H_1 with respect to the eigen-state $|\pm, \vec{n}\rangle$ is

$$E(\pm, \vec{n}) = N(\vec{n})\omega + 2\xi \sum_k n(k) \cos k + \mathcal{C} \qquad (12)$$

with

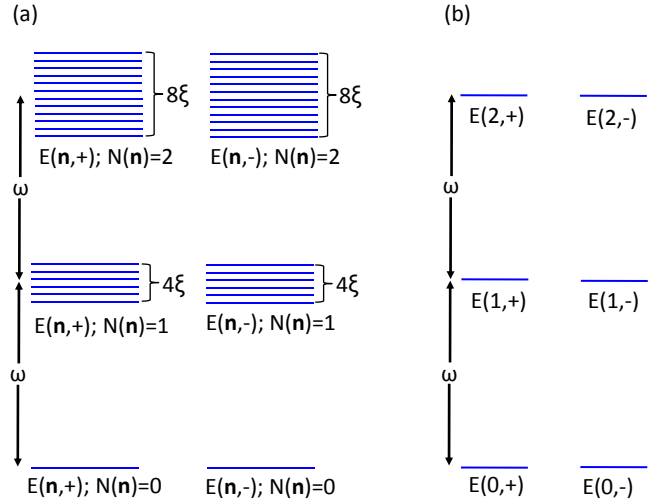$$N(\vec{n}) = \sum_k n(k). \qquad (13)$$

FIG. 2: (Color online) (a) The energy spectrum of the Hamiltonian H_1 of the 1D resonator-array and the interaction between the resonator-array and the TLS. The low-excited spectrum has clear band structure. The intra-band transitions are missed unreasonably in the adiabatic approximation. (b) The energy spectrum of the Hamiltonian H_1 of a single-mode bosonic field and the interaction between the single-mode bosonic field and a TLS. In such a simple system there is no band structure in the spectrum of H_1, and then the adiabatic approximation is applicable when $\Omega << \omega$.

As shown in Fig. 2(a), in the weak-tunneling case with $\xi << \omega$ the low-excited spectrum $E(\pm, \vec{n})$ of the eigen-energies of H_1 has a clear band structure. Each energy band includes all the energy levels with the same total photon number $N(\vec{n})$ and different photon-momentum distribution $\vec{n}$. The N-th energy band is centered at $N\omega$ with band width $4N\xi$. Therefore, in the low excitation cases the inter-band energy gap has the same order with ω.

The spirit of the adiabatic approximation [63–65] is that, during the quantum evolution, the motion of the slowly-varying part of the system would follow the motion of the fast-varying one. Then the quantum state of the fast-varying 1D resonator array would be frozen in each adiabatic branch with fixed quantum number $\vec{n}$. Mathematically speaking, in the adiabatic approximation for our system, all the H_2-induced quantum transitions between the states $|\pm, \vec{n}\rangle$ and $|\pm, \vec{n'}\rangle$ with $\vec{n} \neq \vec{n'}$ are neglected. This treatment leads to the approximate eigen-states of the Hamiltonian H as

$$|\Psi_{\pm, \vec{n}}\rangle = \frac{1}{\sqrt{2}} (|+, \vec{n}\rangle \pm |-, \vec{n}\rangle). \qquad (14)$$

Now we point out that, the adiabatic approximation is *not* a reasonable approximation for our present system, even in the case of $\Omega << \omega$. That is because, the energy spectrum of H_1 has a band structure, each band includes all the states $|\pm, \vec{n}\rangle$ with the same total photon number $N(\vec{n})$. On the other hand, in the adiabatic approxima-

tion all the H_2-induced transitions between the eigenstates of H_1 with different quantum number $\vec{n}$ are neglected. It means that, all the inter-band transitions and the intra-band transitions between the states $|+,\vec{n}\rangle$ and $|-,\vec{n}'\rangle$ with $\vec{n} \neq \vec{n}'$ are omitted. In the case of $\Omega << \omega$, the omission of inter-band transitions are reasonable because the energy gap between different bands is of the order of ω, which is much larger than the intensity Ω of H_2. However, the neglecting of the intra-band transitions are unreasonable because the energy gaps between the levels in the same band can be arbitrary small.

As a comparison, we re-consider the simple system with a single-mode bosonic field interacting with a TLS. In Fig. 2(b), we plot the spectrum of the Hamiltonian

$$H_{\text{Rabi}1} = \omega a^\dagger a + \lambda \sigma_x (a + a^\dagger) \tag{15}$$

with $(a, a^\dagger)$ the annihilation and creation operators of the bosonic field. It is apparent that in such a simple case the spectrum of $H_{\text{Rabi}1}$ does not have any band structure (shown in appendix A). Therefore the adiabatic approximation [58] is applicable when $\Omega << \omega$.

Although the adiabatic approximation cannot be used in our system, as shown in the next subsection, we can still develop the GRWA approach for our system with the help of the basis $\{|\Psi_{\pm,\vec{n}}\rangle\}$. Furthermore, in our GRWA approach the above intrinsic problem of the adiabatic approximation is naturally overcome.

C. The GRWA approach for the TLS-coupled 1D resonator array

Now we develop the GRWA approach for the system of the TLS-coupled 1D resonator array. Similar to the original GRWA for the single-mode bosonic field coupled to a TLS (appendix A), our general GRWA approach can also be considered as an improvement of the adiabatic approximation.

In our GRWA approach the total Hamiltonian H is approximated as H_G which is defined as

$$\begin{aligned} H_G = &\sum_{\vec{n},\vec{n}'} \sum_{\alpha=+,-} H_{\vec{n}',\alpha}^{\vec{n},\alpha} |\Psi_{\alpha,\vec{n}}\rangle\langle\Psi_{\alpha,\vec{n}}| \delta_{N(\vec{n}),N(\vec{n}')} \\ &+ \sum_{\vec{n},\vec{n}'} H_{\vec{n}',-}^{\vec{n},+} |\Psi_{+,\vec{n}}\rangle\langle\Psi_{-,\vec{n}'}| \delta_{N(\vec{n}),N(\vec{n}')-1} + h.c., \end{aligned} \tag{16}$$

where the matrix elements $H_{\vec{n}',\beta}^{\vec{n},\alpha}$ are defined as

$$H_{\vec{n}',\beta}^{\vec{n},\alpha} = \langle\Psi_{\alpha,\vec{n}}|H|\Psi_{\beta,\vec{n}'}\rangle \tag{17}$$

while the symbol $\delta_{a,b}$ is defined as $\delta_{a,b} = 1$ for $a = b$ and $\delta_{a,b} = 0$ for $a \neq b$.

Apparently, in the approximate Hamiltonian H_G we only take into account the quantum transitions between the states $|\Psi_{\alpha,\vec{n}}\rangle$ and $|\Psi_{\beta,\vec{n}'}\rangle$ with

$$N(\vec{n}) + N_\alpha = N(\vec{n}') + N_\beta \tag{18}$$

with $N_\alpha = 1$ for $\alpha = +$ and $N_\alpha = 0$ for $\alpha = -$. Obviously, this treatment is a direct generalization of the one in the development of the GRWA for the TLS-coupled single-mode bosonic field (shown in appendix A).

Furthermore, as proved in appendix C, we have

$$H_{\vec{n}',+}^{\vec{n},-} = 0 \quad \text{for} \quad N(\vec{n}) = N(\vec{n}'). \tag{19}$$

Then the intra-band transition only occurs between the states $|\Psi_{\alpha,\vec{n}}\rangle$ and $|\Psi_{\alpha,\vec{n}'}\rangle$ with $N(\vec{n}) = N(\vec{n}')$. Therefore, all the intra-band transitions, which are unreasonably neglected in the adiabatic approximation, are included in our GRWA approach through the first term of the right hand side of Eq. (16). Thus the intrinsic problem of the adiabatic approximation is overcome in our GRWA approach. Therefore, our approach is applicable in the far-off resonance cases with $\Omega << \omega$.

On the other hand, it is easy to prove that, under the near-resonance condition $\Omega \sim \omega$ and weak-coupling condition $|\lambda| << \omega$, our GRWA approach returns to the rotating-wave approximation. Therefore, as shown in Sec. III, our approach is applicable in a broad parameter region with $\Omega \lesssim \omega$.

Finally, we point out that, the approximate Hamiltonian H_G in the GRWA approach in our case can also be re-expressed in a simple form

$$H_G = U H_R^{\text{RWA}} U^{-1} \tag{20}$$

with U given by Eq.(9) and H_R^{RWA} defined as

$$H_R^{\text{RWA}} \equiv \sum_{n=0}^{\infty} \left[\hat{P}_n \left(U^{-1} H U \right) \hat{P}_n \right]. \tag{21}$$

Here the operator $\hat{P}_n$ is defined as

$$\hat{P}_n = \begin{cases} |0\rangle\langle 0| \otimes |g\rangle\langle g|, & n = 0 \\ \sum_{\{m_l\}} \prod_l |m_l\rangle_l\langle m_l| \otimes |g\rangle\langle g|\delta_{\sum_l m_l, n} + \\ \sum_{\{m_l\}} \prod_l |m_l\rangle_l\langle m_l| \otimes |e\rangle\langle e|\delta_{\sum_l m_l, n-1}, \\ & n \neq 0 \end{cases}$$

where $|m_l\rangle_l$ is the Fock state of the l-th resonator with m_l photons. It is apparent that $\hat{P}_n$ is the projection operator to the eigen-space of the total excitation operator

$$|e\rangle\langle e| + \sum_{j=-\infty}^{+\infty} a_j^\dagger a_j \tag{22}$$

with respect to eigen-value n. In this sense, similarly to the GRWA for the TLS-coupled single-mode bosonic field discussed in appendix A, our GRWA approach can also be considered as "the rotating-wave approximation for the rotated Hamiltonian $U^{-1}HU$".

III. THE SINGLE-PHOTON SCATTERING AMPLITUDES

In the above section we generalize the GRWA to the hybrid system with a 1D resonator array coupled to a single TLS. The single-photon scattering amplitudes in such a system have been calculated analytically under the rotating-wave approximation [2]. In this section we calculate the single-photon scattering amplitudes with our GRWA approach which is applicable in a broader parameter region.

A. The single-photon scattering amplitudes

The single-photon scattering amplitudes can be extracted from the asymptotic behavior of the eigen-state of the Hamiltonian H, which is approximated as H_G in our GRWA approach. To this end, we need to solve the eigen-equation

$$H_G|\Psi(k)\rangle = E(k)|\Psi(k)\rangle \tag{23}$$

with boundary conditions

$$
\begin{aligned}
|\Psi(k)\rangle &= \left(e^{ik(-j)} + r_k e^{-ik(-j)}\right)|1\rangle_{-j}|0\rangle_j|\Phi'(k)\rangle \\
&\quad + t_k e^{ikj}|0\rangle_{-j}|1\rangle_j|\Phi'(k)\rangle + |0\rangle_{-j}|0\rangle_j|\Phi(k)\rangle
\end{aligned}
\tag{24}
$$

in the limit of $j \to +\infty$. Here $|0\rangle_{-j}|0\rangle_j$ is the vacuum state of the resonator modes in the j-th and $-j$-th resonator, $|1\rangle_{-j}|0\rangle_j$ and $|0\rangle_{-j}|1\rangle_j$ are defined as $a_{-j}^\dagger|0\rangle_{-j}|0\rangle_j$ and $a_j^\dagger|0\rangle_{-j}|0\rangle_j$ respectively. $|\Phi(k)\rangle$ and $|\Phi'(k)\rangle$ are the quantum states of the TLS and other resonators except the $\pm j$-th ones. r_k and t_k are the single-photon reflection and transmission amplitudes, or the single-photon scattering amplitudes.

The physical meaning of the boundary condition (24) can be understood as follows: For the scattering state with respect to a single photon input from the left of the 1D resonator array, there are three possible relevant states for the $-j$-th and j-th resonators with large $|j|$, i.e., $|0\rangle_{-j}|0\rangle_j$, $|1\rangle_{-j}|0\rangle_j$ and $|0\rangle_{-j}|1\rangle_j$. Furthermore, the possibility amplitude with respect to $|1\rangle_{-j}|0\rangle_j$ is $\left(e^{ik(-j)} + r_k e^{-ik(-j)}\right)$, since the photon in the $-j$-th resonator can be either the input one or the reflected one. Similarly, the possibility amplitude with respect to $|0\rangle_{-j}|1\rangle_j$ is $t_k e^{ikj}$. It is easy to prove that the boundary condition used in the calculation of the single-photon scattering state with rotating-wave approximation (Eq. (5) of Ref. [2]) can be re-expressed as the one in Eq. (24).

Usually the expression of H_G in Eq. (20) is complicated and the eigen-equation (23) is difficult to be solved directly. However, due to Eq. (20), the Hamiltonian H_G is related to H_R^{RWA} through a unitary transformation. Then the eigen-equation (23) of H_G is equivalent to the

one of H_R^{RWA}:

$$H_R^{\mathrm{RWA}}|\Psi_R(k)\rangle = E(k)|\Psi_R(k)\rangle \tag{25}$$

and the eigen-state $|\Psi_R(k)\rangle$ of H_R^{RWA} is given by

$$|\Psi_R(k)\rangle = U^{-1}|\Psi(k)\rangle. \tag{26}$$

More importantly, with the help of Eq.(9) and the fact that $\lim_{|j|\to\infty}\alpha_j = 0$, the boundary condition (24) for $|\Psi(k)\rangle$ is transformed to the one of $|\Psi_R(k)\rangle$, i.e., in the limit of $j \to \infty$ we have

$$
\begin{aligned}
|\Psi_R(k)\rangle &= \left(e^{ik(-j)} + r_k e^{-ik(-j)}\right)|1\rangle_{-j}|0\rangle_j|\Phi'_R(k)\rangle \\
&\quad + t_k e^{ikj}|0\rangle_{-j}|1\rangle_j|\Phi'_R(k)\rangle + |0\rangle_{-j}|0\rangle_j|\Phi_R(k)\rangle,
\end{aligned}
\tag{27}
$$

where $|\Phi_R(k)\rangle$ and $|\Phi'_R(k)\rangle$ are defined as

$$|\Phi_R(k)\rangle = \prod_{i\neq\pm j}\exp[-\alpha_i\sigma_x(a_i^\dagger - a_i)]|\Phi(k)\rangle, \tag{28}$$

and

$$|\Phi'_R(k)\rangle = \prod_{i\neq\pm j}\exp[-\alpha_i\sigma_x(a_i^\dagger - a_i)]|\Phi'(k)\rangle. \tag{29}$$

respectively. Therefore, the scattering amplitudes r_k and t_k can be obtained from the solution of the eigen-equation (25) of H_R^{RWA} with boundary conditions (27).

B. The perturbative approach for the single-phton scattering amplitudes

In this subsection we solve the eigen-equation (25) of H_R^{RWA} and calculate the single-photon scattering amplitudes. To this end, we first use the explicit result about the unitary operator U shown in appendix B to calculate the Hamiltonian $U^{-1}HU$. We have the results as:

$$
\begin{aligned}
U^{-1}HU &= \omega\sum_{j=-\infty}^{\infty}a_j^\dagger a_j - \xi\sum_{j=-\infty}^{\infty}(a_j^\dagger a_{j+1} + H.c.) \\
&\quad + \frac{\Omega}{2}\left[\cosh(\sum_i 2\nu_i)\sigma_z - i\sinh(\sum_i 2\nu_i)\sigma_y\right]
\end{aligned}
\tag{30}
$$

with $\nu_i = -\alpha_i(a_i^\dagger - a_i)$. In principle, we can derive the explicit expression of H_R^{RWA} with Eqs. (21) and (30). Here, for simplicity, we expand H_R^{RWA} as a power series of the parameter ξ/ω and only keep the low-order terms under the weak-hopping condition $\xi \ll \omega$. Then we can analytically solve Eq. (25) with the approximated H_R^{RWA} and derive the single-photon scattering amplitudes.

Now we calculate the single-photon scattering amplitudes with first-order approximation where only the 0-th order and 1-st order terms of ξ/ω are kept in H_R^{RWA}. As shown in the following, in most of the cases, this approximation is enough to give accurate results for the scattering amplitudes. The straightforward calculation shows

that, up to the first order of ξ/ω, H_R^{RWA} is approximated as

$$
\begin{aligned}
H_R^{\mathrm{RWA}} &\approx H_R^{\mathrm{RWA}(1)} \\
&\equiv \omega \sum_j a_j^\dagger a_j - \xi \sum_j (a_{j+1}^\dagger a_j + h.c.) \\
&\quad + \omega_{0g}^{(0)} (|0g\rangle\langle 0g| + \sum_{j\neq 0} |1_j g\rangle\langle 1_j g|) + \omega_{0e}^{(0)} |0e\rangle\langle 0e| \\
&\quad + \omega_{1g}^{(0)} |1_0 g\rangle\langle 1_0 g| + J^{(0)} (|0e\rangle\langle 1_0 g| + h.c.) \\
&\quad + \omega_{1g}^{(1)} (|1_1 g\rangle\langle 1_0 g| + |1_{-1} g\rangle\langle 1_0 g| + h.c.) \\
&\quad + J^{(1)} (|0e\rangle\langle 1_1 g| + |0e\rangle\langle 1_{-1} g| + h.c.) \qquad (31)
\end{aligned}
$$

with the parameters

$$
\omega_{0g}^{(0)} = -\omega_{0e}^{(0)} = -\frac{\Omega}{2} \exp\left(-2\frac{\lambda^2}{\omega^2}\right); \qquad (32a)
$$

$$
\omega_{1g}^{(0)} = -\frac{\Omega}{2} \exp\left(-2\frac{\lambda^2}{\omega^2}\right)\left(1 - 4\frac{\lambda^2}{\omega^2}\right); \qquad (32b)
$$

$$
J^{(0)} = \frac{\Omega\lambda}{\omega} \exp\left(-2\frac{\lambda^2}{\omega^2}\right); \qquad (32c)
$$

$$
\omega_{1g}^{(1)} = \frac{2\Omega\lambda^2\xi}{\omega^3} \exp\left(-2\frac{\lambda^2}{\omega^2}\right); \qquad (32d)
$$

$$
J^{(1)} = \frac{\Omega\lambda\xi}{\omega^2} \exp\left(-2\frac{\lambda^2}{\omega^2}\right). \qquad (32e)
$$

In Eq. (31) the states $|0e\rangle$, $|0g\rangle$, $|1_j e\rangle$ and $|1_j g\rangle$ are defined as $|0\rangle|e\rangle$, $|0\rangle|g\rangle$, $|1_j\rangle|e\rangle$ and $|1_j\rangle|g\rangle$ respectively, where $|0\rangle$ is the vacuum state of all the resonators.

The physical meaning of Eq. (31) is very clear. In the 0-th order terms of ξ/ω, or the terms proportional to $\omega_{0g}^{(0)}$, $\omega_{0e}^{(0)}$, $\omega_{1g}^{(0)}$ and $J^{(0)}$, the effective couplings occur between

the TLS and the photon in the 0-th resonator in which the TLS is located. Nevertheless, in the 1-st order terms proportional to $J^{(1)}$, effective couplings appear between the TLS and the modes in the ± 1-st resonators. These terms imply that the non-rotating-wave effects from the coupling between the TLS and the 0-th resonator can indirectly influence the behavior of the modes in the ± 1-st resonators. Furthermore, the hopping intensities between the 0-th and ± 1-st resonators are also tuned by the terms with $\omega_{1g}^{(1)}$.

As shown above, the single-photon scattering amplitudes are approximately derived from the eigen-equation

$$
H_R^{\mathrm{RWA}(1)} |\Psi_R(k)\rangle = E(k) |\Psi_R(k)\rangle \qquad (33)
$$

of $H_R^{\mathrm{RWA}(1)}$ with boundary condition (27). It is apparent that the solution $|\Psi_R(k)\rangle$ of Eq.(33) takes the form

$$
|\Psi_R(k)\rangle = \sum_{j=-\infty}^{+\infty} u_k^{(1)}(j) |1_j g\rangle + u_e^{(1)} |0e\rangle \qquad (34)
$$

with the coefficients $u_k^{(1)}(j)$ given by

$$
u_k^{(1)}(j) = \begin{cases} e^{ikj} + r_k^{(1)} e^{-ikj}, & j \leqslant -1 \\ u_k(0), & j = 0 \\ t_k^{(1)} e^{ikj}. & j \geqslant 1 \end{cases} \qquad (35)
$$

Substituting Eqs.(34,35) into Eq.(33), we obtain the linear equations for the reflection amplitude $r_k^{(1)}$ and transmission amplitude $t_k^{(1)}$. These equations can be solved analytically. Then we obtain the scattering amplitudes $r_k^{(1)}$ and $t_k^{(1)}$ given by the first-order approximation of H_R^{RWA}:

$$
r_k^{(1)} = \frac{e^{ik}\lambda^2\Omega \left\{ \begin{array}{c} 4\lambda^2\xi\Omega^2\cos(k) + 2e^{\frac{4\lambda^2}{\omega^2}}\omega^3\left[\omega^2 + 2\xi\omega\cos(k) - 4\xi^2 - 4\xi^2\cos(2k)\right] \\ +e^{\frac{2\lambda^2}{\omega^2}}\Omega\left[8\lambda^2\xi^2 + 2\omega^2\xi^2 - \omega^4 - 4\xi\omega\left(2\lambda^2 + \omega^2\right)\cos(k) + 2\xi^2\left(4\lambda^2 + \omega^2\right)\cos(2k)\right] \end{array} \right\}}{\left\{ \begin{array}{c} -4e^{2ik}\lambda^4\xi\Omega^3 + e^{\frac{6\lambda^2}{\omega^2}}\left(-1 + e^{2ik}\right)\xi\omega^6\left[\omega - 2\xi\cos(k)\right] \\ +e^{\frac{4\lambda^2}{\omega^2}}\omega^3\Omega\left[8e^{3ik}\lambda^2\xi^2 + 2e^{ik}\lambda^2\left(4\xi^2 - \omega^2\right) + \xi\omega\left(2\lambda^2 + \omega^2\right) - e^{2ik}\xi\omega\left(6\lambda^2 + \omega^2\right)\right] \\ +e^{2ik+\frac{\lambda^2}{\omega^2}}\lambda^2\Omega^2\left[4\xi\omega\left(2\lambda^2 + \omega^2\right) + \left(\omega^4 - 4\xi^2\omega^2 - 16\lambda^2\xi^2\right)\cos(k) - i\omega^4\sin(k)\right] \end{array} \right\}}, \qquad (36)
$$

$$
t_k^{(1)} = r_k^{(1)} + 1. \qquad (37)
$$

The above procedure can be straightforwardly generalized to the cases with high-order approximations of H_R^{RWA}. For instance, in the second-order approximation, H_R^{RWA} is approximated as $H_R^{\mathrm{RWA}(2)}$ which includes the 0-th order, 1-st order and 2-nd order terms of ξ/ω. It can be found that in $H_R^{\mathrm{RWA}(2)}$ the TLS is effectively coupled to the 0-th, ± 1-st and ± 2-nd resonators. We can also

solve the eigen-equation of $H_R^{\mathrm{RWA}(2)}$, and obtain the analytical expressions of the relevant scattering amplitudes $r_k^{(2)}$ and $t_k^{(2)}$. In general, for any integer n, the scattering amplitudes $r_k^{(n)}$ and $t_k^{(n)}$ from the n-th order approximation of H_R^{RWA} can be obtained with the similar approach. In the limit of $n \to \infty$, the results $r_k^{(n)}$ and $t_k^{(n)}$ would
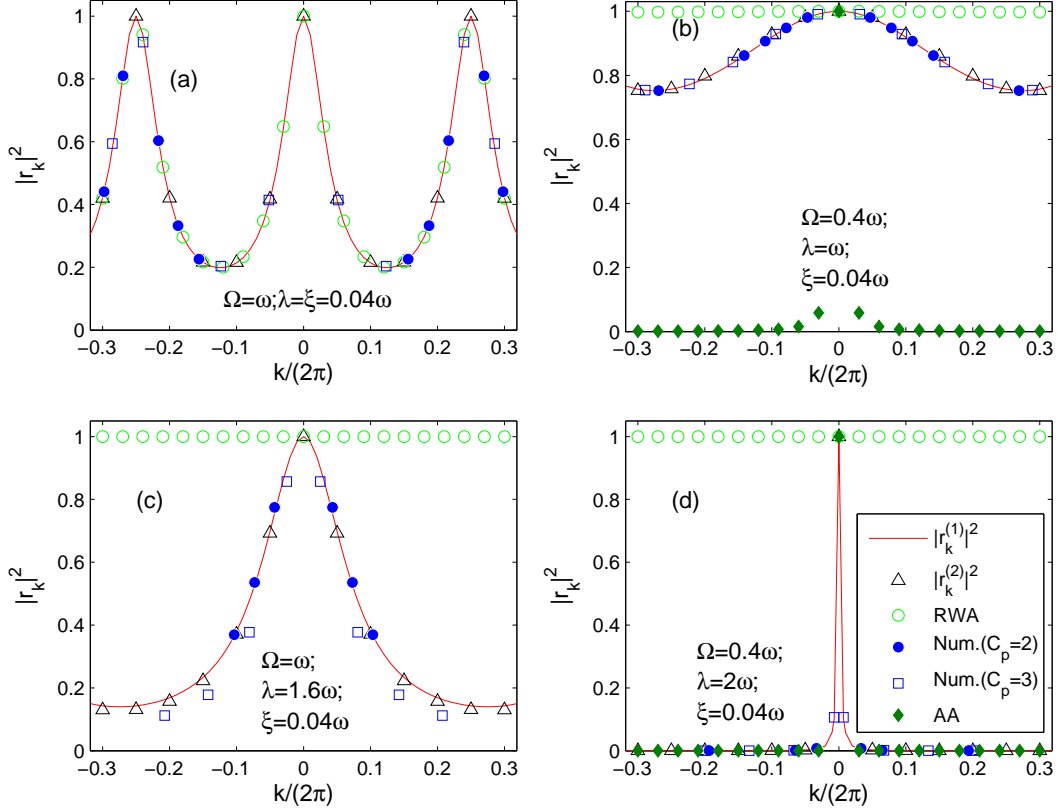
FIG. 3: (Color online) The single-photon reflection rate $|r_k|^2$ given by our GRWA approach with the first and second order approximation for (ξ/ω), i.e., $|r_k^{(1)}|^2$ (red solid line) and $|r_k^{(2)}|^2$ (black empty triangle), $|r_k|^2$ from the rotating-wave approximation (RWA) (green empty circle), $|r_k|^2$ from the adiabatic approximation (green filled diamond) and the numerical calculations with cut-off excitation number $C_p = 2$ (blue filled circle) and $C_p = 3$ (blue empty square). Here we consider the cases of $\xi = 0.04\omega$ and $\Omega = \omega$, $\lambda = 0.04\omega$ (a), $\Omega = 0.4\omega$, $\lambda = \omega$ (b), $\Omega = \omega$, $\lambda = 1.6\omega$ (c) and $\Omega = 0.4\omega$, $\lambda = 2\omega$ (d).

converge to fixed values r_k and t_k or the precise values of the single-photon scattering amplitudes.

C. Results and discussions

In Figs. 3 and 4, we illustrate the single-photon scattering amplitude r_k given by our GRWA approach with the first and second order approximations, i.e., $r_k^{(1)}$ and $r_k^{(2)}$, the one given by the rotating-wave approximation and the result from the numerical diagonalization of the rotated Hamiltonian $U^{-1}HU$. In our numerical calculations the total excitation defined in (22) is cut off at a given number C_p for the Hamiltonian $U^{-1}HU$, and the results with $C_p = 2$, 3 are shown in our figures.

In Fig. 3 we calculate the reflection rate $|r_k|^2$. It is clearly shown that the results $|r_k^{(1)}|^2$ and $|r_k^{(2)}|^2$ from the first and second order approximation for (ξ/ω) consist very well with each other. Therefore, in most of the cases with $|\xi| \ll \omega$, the first order approximation is good enough for our GRWA approach.

Furthermore, it is shown that in the case of Fig. 3(a) where the weak-coupling and near-resonance conditions

are satisfied, both the results from the rotating-wave approximation and our GRWA approach fit well with the numerical calculations. Nevertheless, in the cases of Figs. 3(b)-3(d) where the rotating-wave approximation is not applicable, the results from our GRWA approach also consist significantly well with the numerical calculations. This observation is further confirmed by Fig. 4 where the real and imaginary parts of r_k given by different approaches are illustrated.

In Figs. 3(b) and 3(d) with $\Omega = 0.4\omega$, we also compare our results with the ones given by the adiabatic approximation. It is shown that as we argued in Sec. II, the adiabatic approximation may be not applicable even when $\Omega \ll \omega$, while our GRWA approach can still provide reasonable results.

Therefore, the results in Figs. 3 and 4 show that, our GRWA approach with the first-order approximation for (ξ/ω), or our results $r_k^{(1)}$ and $t_k^{(1)}$ in Eqs. (36, 37) can be used as a good analytical approximation for the single-photon scattering amplitudes in the parameter region with $|\xi| \ll \omega$ and $\Omega \lesssim \omega$.
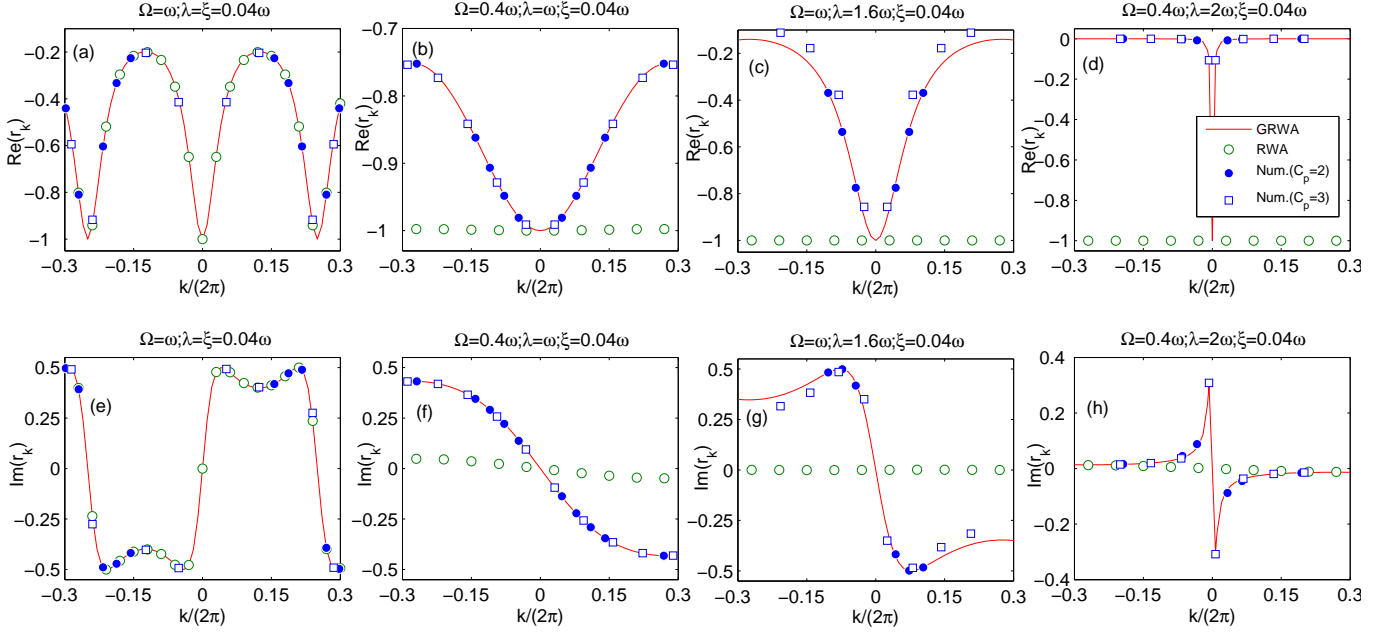
FIG. 4: (Color online) The real parts (a-d) and imaginary parts (e-h) of the single-photon scattering amplitude r_k given by our GRWA approach with the first-order approximation for (ξ/ω), i.e., $r_k^{(1)}$ in Eq.(36) (red solid line), the rotating-wave approximation (green empty circle) and the numerical calculations with cut-off excitation number $C_p = 2$ (blue filled circle) and $C_p = 3$ (blue empty square). Here we consider the cases of $\xi = 0.04\omega$ and $\Omega = \omega$, $\lambda = 0.04\omega$ (a, e), $\Omega = 0.4\omega$, $\lambda = \omega$ (b, f), $\Omega = \omega$, $\lambda = 1.6\omega$ (c, g) and $\Omega = 0.4\omega$, $\lambda = 2\omega$ (d, h).

IV. THE SCATTERING AMPLITUDES IN THE STRONG-COUPLING CASE

In the above section we derived the single-photon scattering amplitudes with our GRWA approach. It is pointed out that, our results in Eqs. (32a-32e) are applicable for arbitrary large coupling between the TLS and the photon. Now we consider a special case where the TLS is strongly coupled to the photon in the resonator array, so that the condition

$$\frac{\lambda^2}{\omega^2} e^{-2\frac{\lambda^2}{\omega^2}} << 1 \qquad (38)$$

is satisfied. We further assume the frequency Ω of the TLS is equal to or smaller than the photon frequency ω, i.e., $\Omega \lesssim \omega$. In this strong-coupling case the expressions in Eqs. (32a-32e) can be significantly simplified and then one obtains simple pictures for both the quantitative calculation and the qualitative estimation of the single-photon scattering amplitudes.

Under the condition (38), we only keep the leading term proportional to $\left(\lambda^2/\omega^2\right) \exp\left(-2\lambda^2/\omega^2\right)$ in $\omega_{0g,e}^{(0)}$, $\omega_{1g}^{(0,1)}$ and $J^{(0,1)}$ defined in Eqs. (32a-32e). Then we have

$$\omega_{1g}^{(0)} \approx \frac{2\Omega\lambda^2}{\omega^2} \exp\left(-2\frac{\lambda^2}{\omega^2}\right), \qquad (39a)$$

$$\omega_{1g}^{(1)} \approx \frac{\xi}{\omega}\omega_{1g}^{(0)}, \qquad (39b)$$

$$\omega_{0g,e}^{(0)}, \ J^{(0,1)} \approx 0. \qquad (39c)$$

Therefore, in Eq.(31) of the Hamiltonian H_R^{RWA}, we only need to keep the first two terms and the terms proportional to $\omega_{1g}^{(0)}$ and $\omega_{1g}^{(1)}$. This simplification implies that, in the strong-coupling regime our system is equivalent to the simple 1D resonator array with the frequency of the 0-th resonator shifted from ω to $\omega + \omega_{1g}^{(0)}$, while the photonic hopping intensity between the 0-th resonator and the ±1-st ones shifted from ξ to $\xi + \omega_{1g}^{(1)}$. Since we have also assumed $\Omega \lesssim \omega$, it is apparent that $\omega_{1g}^{(1)} << \xi$ in the strong-coupling regime. Then the shift $\omega_{1g}^{(1)}$ of the photonic hopping intensity is negligible. We only need to consider the effect given by the frequency shift $\omega_{1g}^{(0)}$ of the photon in the 0-th resonator. Namely, our system is finally equivalent to a 1D resonator array, in which the 0-th resonator has the frequency $\omega + \omega_{1g}^{(0)}$, while all the other resonators have the same frequency ω. In this case the Hamiltonian $H_R^{\mathrm{RWA}(1)}$ is approximated as

$$H_R^{\mathrm{RWA}(1)} \approx \omega \sum_j a_j^\dagger a_j - \xi \sum_j \left(a_{j+1}^\dagger a_j + a_j^\dagger a_{j+1}\right) + \omega_{1g}^{(0)} a_0^\dagger a_0, \qquad (40)$$

which leads to the single-photon scattering amplitudes

$$r_k \approx -\frac{\omega_{1g}^{(0)}}{\omega_{1g}^{(0)} - 2i\xi \sin(k)}, \qquad (41)$$
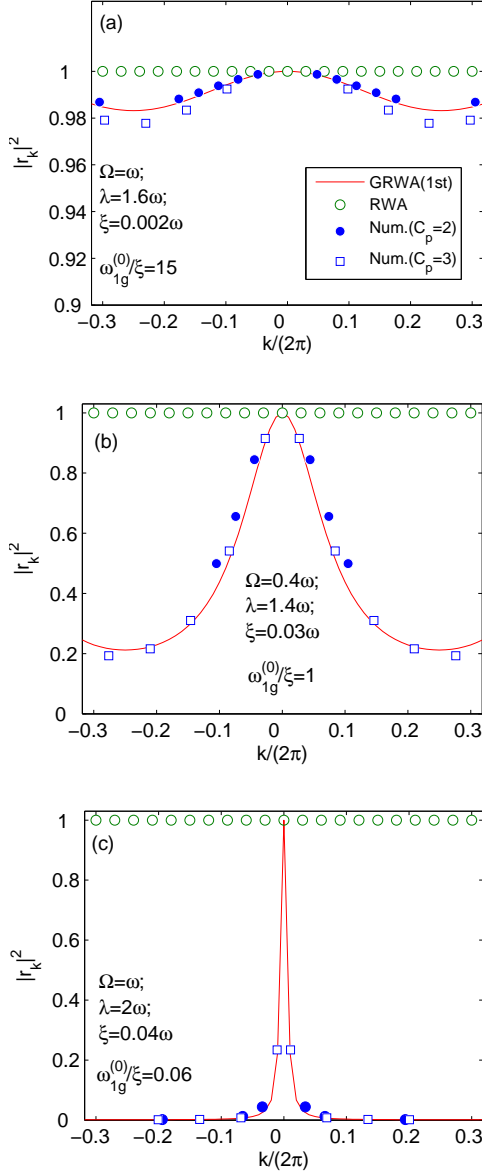
$$t_k \approx r_k + 1. \qquad (42)$$

FIG. 5: (Color online) The single-photon reflection rate $|r_k|^2$ in the cases with strong TLS-photon coupling. Here we show the results given by Eq.(41) (red solid line), rotating-wave approximation (green empty circle) and the numerical calculations with cut-off excitation number $C_p = 2$ (blue filled circle) and $C_p = 3$ (blue empty square) for the cases with $\Omega = \omega$, $\lambda = 1.6\omega$, $\xi = 0.002\omega$ (a), $\Omega = 0.4\omega$, $\lambda = 1.4\omega$, $\xi = 0.03\omega$ (b), $\Omega = \omega$, $\lambda = 2\omega$, $\xi = 0.04\omega$ (c). In the three cases we have $\omega_{1g}^{(0)}/\xi = 15, 1, 0.06$ respectively.

A straightforward result given by the above expressions of the scattering amplitudes is that, when the effective frequency shift $\omega_{1g}^{(0)}$ of 0-th resonator is much larger than the band width 4ξ of the free Hamiltonian H_C of the array of resonators with the same frequency ω, the 0-th resonator would be far-off detuned with the photon with any incident momentum k, and then every photon would be reflected. Namely, in such a limit we have $r_k \approx 1$, $t_k \approx 0$. Likewise, if the effective frequency shift $\omega_{1g}^{(0)}$ is much smaller than 4ξ, the frequency of the 0-th resonator would be approximately the same as the other resonators, and then every photon transmits through the 0-th resonator. In this limit we have $r_k \approx 0$ and $t_k \approx 1$.

In Fig. 5 we plot the photon reflection rate $|r_k|^2$ in the strong-coupling cases and compare the results given by our result in Eq. (41) and the one from numerical diagonalization of the rotated Hamiltonian $U^{-1}HU$ with cut-off excitation number $C_p = 2, 3$ respectively. It is clearly shown that our results in Eq. (41) fit well with the numerical results. Furthermore, it is illustrated that in the case of Fig. 5(a) where we have $\omega_{1g}^{(0)}/\xi = 15$, the photon reflection rate $|r_k|^2$ is almost unit for all the incident momentum k. In the case of Fig. 5(c) with $\omega_{1g}^{(0)}/\xi = 0.06$, we have $|r_k|^2 \approx 0$ in the region with non-zero momentum k. All these observations are consistent with our above qualitative analysis.

In the end of this section, we remark that, since all the quantities defined in Eqs. (32a-32e) exponentially decay to zero with (λ/ω), for any given values of Ω, ω and ξ, when the TLS-photon coupling intensity λ is large enough, we can always neglect all these parameters and approximate the Hamiltonian $H_R^{\text{RWA}(1)}$ as the free Hamiltonian H_C for the array of identical resonators. Therefore, when the TLS-photon coupling is strong enough, the photonic scattering effect becomes negligible and we have $r_k = 0$, $t_k = 1$ for the photon with any incident momentum k.

V. THE GRWA FOR RESONATOR ARRAY WITH MULTI TLSS

In the above sections, we generalized the GRWA to the system with 1D resonator array coupled to a single TLS, and calculated the single-photon scattering amplitudes with the GRWA approach. In the end of this paper, we extend the GRWA to more general cases with m two-level systems coupled to the resonator array. For simplicity, here we assume each TLS is individually located in a resonator. Then the Hamiltonian of the total system is written as

$$H_M = H_C + H_{AM} + H_{IM} \qquad (43)$$

with the Hamiltonian H_C of the resonator defined in Eq. (1), the Hamiltonian H_{AM} of all the TLSs given by

$$H_A = \frac{\Omega}{2} \sum_{\beta=1}^{m} \sigma_z^{(\beta)} \qquad (44)$$

and the interaction Hamiltonian H_{IM} defined as

$$H_{IM} = \lambda \sum_{\beta=1}^{m} \sigma_x^{(\beta)} \left(a_{c(\beta)}^\dagger + a_{c(\beta)} \right). \qquad (45)$$

Without loss of generality, here we assume the β-th TLS is located in the $c(\beta)$-th resonator.

In such a general system, we straightforwardly develop the GRWA approach with the unitary transformation procedure in Sec. II and Sec. III. To this end, we first write the Hamiltonian H_M as

$$H_M = H_{M1} + H_{M2}$$

with H_{M1} and H_{M2} defined as

$$H_{M1} = H_C + H_{IM}, \qquad (46)$$
$$H_{M2} = H_{AM}. \qquad (47)$$

Then we should find a unitary operator U_M which can eliminate the linear terms of $(a_j, a_j^\dagger)$ in H_{M1} and satisfies

$$U_M^{-1} H_{M1} U_M$$
$$= \omega \sum_{j=-\infty}^{\infty} a_j^\dagger a_j - \xi \sum_{j=-\infty}^{\infty} (a_j^\dagger a_{j+1} + h.c.) - \mathcal{C}_M \quad (48)$$

with $\mathcal{C}_M$ a constant c-number. The analytical calculation of U_M is obtained in appendix D.

With the operator U_M, we apply the unitary transformation to the total Hamiltonian H, and make the rotating-wave approximation to the transformed Hamiltonian $U_M^{-1} H_M U_M$. Finally we perform the inverse unitary transformation. Then the GRWA Hamiltonian for the resonator array with multi TLSs is obtained as:

$$H_M \approx H_{MG}$$
$$\equiv U_M \left\{ \sum_{n=0}^{\infty} \left[\hat{P}_{Mn} \left(U_M^{-1} H_M U_M \right) \hat{P}_{Mn} \right] \right\} U_M^{-1},$$
$$(49)$$

which is a direct generalization of the result in Eq. (20). Here $\hat{P}_{Mn}$ is the projection operator to the eigen-space of the total excitation operator

$$\sum_{\beta=1}^{m} |e\rangle^{(\beta)}\langle e| + \sum_{j=-\infty}^{+\infty} a_j^\dagger a_j \qquad (50)$$

with respect to eigen-value n. It is straightforwardly observed that, in the case of $\Omega << \omega$, such an approach also includes the intra-band transitions which are missed in the adiabatic approximation. On the other hand, under the weak-coupling condition and near-resonance condition, this approach converges to the rotating-wave approximation.

VI. CONCLUSIONS

In conclusion we generalize the GRWA to the hybrid system of a 1D single-mode resonator array coupled to a single TLS, and obtain the analytical results for the single-photon scattering amplitudes under the conditions $|\xi| << \omega$ and $\Omega \lesssim \omega$. It is shown that in comparison with the rotating-wave approximation, our GRWA approach can give good results in a much broader parameter region. Especially, in the far-off resonance case with $\Omega << \omega$, the adiabatic approximation is no longer applicable for our current system, while our approach still works well. We also generalize our GRWA approach to the 1D resonator array coupled to multi-TLSs.

In this paper, we assume the resonators in the 1D array are single-mode ones. However, in the resonators used in the experiments, there usually exist more than one photon modes. Then in the cases with strong TLS-photon coupling the multi-mode effect may be important. Likewise, it may be also necessary to go beyond the two-level approximation and include the higher excited states of the artifical atoms in the strong-coupling cases. These effects will be discussed in our coming work for the calculation of the photon scattering in an multi-mode-resonators array or a multi-mode wave guide beyond the rotating-wave approximation.

Appendix A: GRWA for the TLS-coupled single-mode bosonic field

In this appendix, we introduce the GRWA approach proposed by Irish in Ref. [57] in the view of adiabatic approximation. To this end, we begin with the simple Rabi Hamiltonian for the TLS-coupled single-mode bosonic field:

$$H_{\text{Rabi}} = \omega a^\dagger a + \frac{\Omega}{2}\sigma_z + \lambda \sigma_x(a^\dagger + a). \qquad (A1)$$

Here a and $a^\dagger$ are the annihilation and creation operators of the single-mode bosonic field with frequency ω respectively. Ω is the energy level spacing between the excited state $|e\rangle$ and the ground state $|g\rangle$ of the TLS, and λ is the coupling intensity between the TLS and the bosonic field. The Pauli operators σ_z and σ_x are defined in Sec. II.

Since the Hamiltonian H_{Rabi} does not have simple invariable subspaces, the exact diagonalization of H_{Rabi} is rather complicated [61]. However, Jaynes and Cumming showed that [62], under the near-resonance condition

$$|\omega - \Omega| << |\omega + \Omega| \qquad (A2)$$

and weak coupling condition

$$|\lambda| << \omega, \Omega, \qquad (A3)$$

the term $|e\rangle\langle g|\, a^\dagger + h.c$ would be safely neglected. Then the Hamiltonian H_{Rabi} is approximated as the H_{JC} which is defined as

$$H_{JC} = \omega a^\dagger a + \lambda(|e\rangle\langle g|a + h.c.). \tag{A4}$$

That is the so called rotating-wave approximation. After this approximation, the Hamiltonian H_{Rabi} becomes invariable in the two-dimensional subspaces spanned by the states $|g,n\rangle$ and $|e, n-1\rangle$ for $n = 1,2,...$, as well as the one-dimensional subspace spanned by $|g, 0\rangle$ and then can be diagonalized easily.

For the convenience of our discussions on the GRWA, here we introduce the projection operators $\hat{P}_{\text{Rabi}}^{(n)}$ defined as

$$\hat{P}_{\text{Rabi}}^{(n)} = \begin{cases} |0g\rangle\langle 0g|, & n = 0 \\ |n,g\rangle\langle n,g| + |n-1,e\rangle\langle n-1,e|, & n \geq 1 \end{cases}. \tag{A5}$$

Then the Jaynes-Cumming Hamiltonian H_{JC} in Eq. (A4) is re-written as

$$H_{JC} = \sum_{n=0}^{\infty} \hat{P}_{\text{Rabi}}^{(n)} H_{\text{Rabi}} \hat{P}_{\text{Rabi}}^{(n)}. \tag{A6}$$

Now we introduce the GRWA approach, which is developed as an analytical approximate method to diagonalize the Hamiltonian H in Eq. (A1) in a broad parameter region where the rotating-wave approximation could be either applicable or not. The GRWA is closely related to both the rotating-wave approximation and the adiabatic approximation [63–65] for the TLS-coupled single-mode bosonic field [57–59] which is used in the case of far-off resonance

$$\Omega << \omega. \tag{A7}$$

Therefore, before introducing the GRWA, we first introduce the adiabatic approximation in the system of a TLS and a single-mode bosonic field[57, 58]. In such an approximation, the bosonic field is considered to be the fast-varying part of the total system and the TLS is considered as the slowly-varying part. Then the Hamiltonian H_{Rabi} is rewritten as

$$H_{\text{Rabi}} = H_{\text{Rabi1}} + H_{\text{Rabi2}}, \tag{A8}$$

where

$$H_{\text{Rabi1}} = \omega a^\dagger a + \lambda \sigma_x (a^\dagger + a) \tag{A9}$$

is the self-Hamiltonian of the fast-varying part together with the interaction between the fast-varying part and the slowly-varying one, and

$$H_{\text{Rabi2}} = \frac{\Omega}{2}\sigma_z \tag{A10}$$

is the self-Hamiltonian of the slowly-varying part.

The Hamiltonian H_{Rabi1} is easily diagonalized with the eigenstates:

$$|\pm, n\rangle = |\pm\rangle \otimes |n_\pm\rangle, \tag{A11}$$

and the relevant eigen-energies:

$$E_{n\pm} = \omega(n - \lambda^2/\omega^2). \tag{A12}$$

Here $|\pm\rangle$ are the eigenstates of σ_x with eigen-values ± 1 and $|n_\pm\rangle$ are defined as

$$|n_\pm\rangle = \exp[\mp\lambda/\omega(a^\dagger - a)]\,|n\rangle. \tag{A13}$$

In the Rabi Hamiltonian the states $|\alpha, n\rangle$ and $|\alpha', n'\rangle$ are coupled by the term H_{Rabi2}.

The spirit of the adiabatic approximation is described as follows [63–65]: under the far-off resonance condition $\Omega << \omega$, the motion of fast-varying part or the bosonic field adiabatically follows the slowly-varying part or the TLS, and can be frozen in the adiabatic branches with fixed quantum number n, or the two-dimensional subspaces spanned by $|+, n\rangle$ and $|-, n\rangle$ for $n = 1, 2, ...$. Then we neglect the H_{Rabi2}-induced transitions between the states $|\alpha, n\rangle$ and $|\alpha', n'\rangle$ with $n \neq n'$. Then the eigenstates and eigen-energies of H are approximated as:

$$|\Psi_{\pm,n}\rangle = \frac{1}{\sqrt{2}}(|+, n\rangle \pm |-, n\rangle), \tag{A14}$$

and

$$E_{\pm,n} = \pm\frac{\Omega}{2}\langle n_-|n_+\rangle + \omega(n - \lambda^2/\omega^2). \tag{A15}$$

respectively.

Now we introduce the GRWA. In the "adiabatic basis" $\{|\Psi_{\pm,n}\rangle\}$, the Hamiltonian H is rewritten as

$$H_{\text{Rabi}} = \sum_{n,n'} \sum_{\alpha,\alpha'=\pm} (H_{\text{Rabi}})_{\alpha,n}^{\alpha',n'} |\Psi_{\alpha,n}\rangle\langle\Psi_{\alpha',n'}| \tag{A16}$$

with the matrix elements

$$(H_{\text{Rabi}})_{\alpha,n}^{\alpha',n'} = \langle\Psi_{\alpha,n}|H_{\text{Rabi}}|\Psi_{\alpha',n'}\rangle. \tag{A17}$$

In the GRWA, the Rabi Hamiltonian H_{Rabi} is approximated as H_{RG} which is defined as

$$\begin{aligned} H_{RG} &= \sum_{n=0}^{+\infty} \sum_{\alpha=\pm} (H_{\text{Rabi}})_{\alpha,n}^{\alpha,n} |\Psi_{\alpha,n}\rangle\langle\Psi_{\alpha,n}| \\ &+ \sum_{n=1}^{\infty} (H_{\text{Rabi}})_{-,n}^{+,n-1} |\Psi_{-,n}\rangle\langle\Psi_{+,n-1}| + h.c.. \end{aligned} \tag{A18}$$

Namely, only the matrix elements $(H_{\text{Rabi}})_{\alpha,n}^{\alpha',n'}$ inside each two-dimensional subspaces spanned by the states $|\Psi_{-,n}\rangle$ and $|\Psi_{+,n-1}\rangle$ as well as the one in the one-dimensional subspace spanned by the state $|\Psi_{-,0}\rangle$ are kept in the GRWA. In other words, in the GRWA one takes into account only the quantum transitions between the states $|\Psi_{\alpha,n}\rangle$ and $|\Psi_{\beta,n'}\rangle$ with

$$n + N_\alpha = n' + N_\beta \tag{A19}$$

with $N_\alpha = 1$ for $\alpha = +$ and $N_\alpha = 0$ for $\alpha = -$. Then, similarly as in the rotating-wave approximation, the Hamiltonian is reduced into a 2×2 blocked diagonal matrix in the GRWA.

It can be shown that, under the weak-coupling and near-resonance conditions, the GRWA returns to the rotating-wave approximation. On the other hand, under the far-off resonance condition, the results given by the GRWA converges to the one from adiabatic approximation. Therefore, the GRWA smoothly connects the ordinary rotating wave approximation and the adiabatic approximation, and then works well in a more broad parameter regime, especially the region with strong TLS-photon coupling and far-off resonant $\Omega \lesssim \omega$ (see, e.g., Ref. [57] and Fig. 8 of Ref. [60]).

In the end of this appendix, we emphasis that, the Hamiltonian H_{RG} defined in (A18) could also be re-written as [57]

$$H_{RG} = U_R \left\{ \sum_{n=0}^{\infty} \left(\hat{P}_n \left(U_R^{-1} H_{\text{Rabi}} U_R \right) \hat{P}_n \right) \right\} U_R^{-1} \quad (A20)$$

with the unitary transformation U_R defined as

$$U_R = \exp\left[-\frac{\lambda}{\omega} \sigma_x (a^\dagger - a) \right]. \quad (A21)$$

Comparing Eq. (A20) and Eq. (A6), one can find that the GRWA is nothing but the "rotating-wave approximation for the rotated Hamiltonian $U_R^{-1} H_{\text{Rabi}} U_R$".

Appendix B: The unitary transformation U

In this appendix, we calculate the unitary transformation U determined by Eq. (9) and Eq. (10). It is obvious that U can be expressed as the product of the displacement operators for each resonator mode, i.e., we have

$$U = \prod_{j=-\infty}^{+\infty} \exp[\alpha_j \sigma_x (a_j^\dagger - a_j)]. \quad (B1)$$

Then the Hamiltonian H_1 is transformed into

$$\begin{aligned} &U^{-1} H_1 U \\ &= H_C + \sum_{j \neq 0} [\omega \alpha_j - \xi(\alpha_{j+1} + \alpha_{j-1})] \sigma_x (a_j^\dagger + a_j) \\ &\quad + [\omega \alpha_0 - \xi(\alpha_1 + \alpha_{-1}) + \lambda] \sigma_x (a_0^\dagger + a_0) - \mathcal{C}. \end{aligned} \quad (B2)$$

The exact expression of $\mathcal{C}$ is not required here. Comparing the result Eq. (B2) with Eq. (8), we get the equations for the parameters $\{\alpha_j\}$:

$$\omega \alpha_j - \xi(\alpha_{j+1} + \alpha_{j-1}) = 0, j = \pm 1, \pm 2, ... \quad (B3)$$
$$\omega \alpha_0 - \xi(\alpha_1 + \alpha_{-1}) + \lambda = 0, j = 0. \quad (B4)$$

Now we solve Eqs. (B3, B4) with two steps. First, we introduce a cut-off for the equations at $j = \pm N$, and solve the equations

$$\omega \alpha_j^{(N)} - \xi \left(\alpha_{j+1}^{(N)} + \alpha_{j-1}^{(N)} \right) = 0, \ j = \pm 1, ..., \pm(N-1) \quad (B5)$$

$$\omega \alpha_0^{(N)} - \xi \left(\alpha_1^{(N)} + \alpha_{-1}^{(N)} \right) + \lambda = 0, \ j = 0, \quad (B6)$$

$$\alpha_N^{(N)} = \alpha_{-N}^{(N)} = 0. \quad (B7)$$

A straightforward calculation shows that

$$\begin{aligned} \alpha_j^{(N)} &= \left[\left(\frac{\omega}{2\xi} - \frac{\xi}{\omega_1} \right) \alpha_0^{(N)} + \frac{\lambda}{2\xi} \right] \frac{(\frac{\xi}{\omega_1})^{|j|-1} - (\frac{\omega_1}{\xi})^{|j|+1}}{1 - (\frac{\omega_1}{\xi})^2} \\ &\quad + (\frac{\xi}{\omega_1})^{|j|} \alpha_0^{(N)} \end{aligned} \quad (B8)$$

with ω_1 given by

$$\omega_1 = \frac{1}{2} \left(\omega + \sqrt{\omega^2 - 4\xi^2} \right). \quad (B9)$$

Therefore, under the weak-hopping assumption $|\xi| << \omega$, we have $\xi/\omega_1 < 1$. Substituting Eq. (B7) into Eq. (B8), we obtain

$$\alpha_0^{(N)} = \frac{-\lambda \omega_1 \left[(\frac{\omega_1}{\xi})^{2|N|} - 1 \right]}{-\omega \omega_1 + 2\omega_1^2 - 2\xi^2(\frac{\omega_1}{\xi})^{2|N|} + \omega \omega_1 (\frac{\omega_1}{\xi})^{2|N|}} \quad (B10)$$

and then we obtain all $\alpha_j^{(N)}$ from Eq. (B8).

Second, we consider the solutions of Eqs. (B5-B7) in limit of $N \to \infty$ as a trial solution of Eqs. (B3, B4):

$$\alpha_j = \lim_{N \to \infty} \alpha_j^{(N)} = \frac{\lambda \omega_1}{2\xi^2 - \omega \omega_1} (\frac{\xi}{\omega_1})^{|j|}. \quad (B11)$$

Substituting Eq. (B11) into Eqs. (B3, B4), we find that the latter ones are exactly satisfied. Therefore, $\{\alpha_j\}$ from Eq. (B11) are the realistic solutions of Eqs. (B3, B4). Then the unitary transformation U defined in Eq. (8) takes the form Eq. (9) with α_j given by Eq. (10).

We emphasis that, as shown in Eq. (B1), U is the product of the displacement operators for each resonator, the magnitude of the displacement for the mode in the j-th resonator is described by $|\alpha_j|$. Furthermore, since $\xi/\omega_1 < 1$, the result Eq. (B11) implies that $|\alpha_j|$ exponentially decays with $|j|$. Then we have

$$\lim_{|j| \to \infty} \exp[\alpha_j \sigma_x (a_j^\dagger - a_j)] = 1 \quad (B12)$$

Therefore, for the resonators which are far away from the TLS, the relevant displacements in U would be negligible, this is consistent with our above considerations.

Appendix C: The proof of Eq. (19)

In this appendix, we prove Eq. (19) in our maintext. To this end, we first define the operator $\mathcal{U}_k[\beta_k]$ and the state $|n(k)\rangle$ for the 1D resonator array as a function of the number β_k:

$$\mathcal{U}_k[\beta_k] = \exp\left\{-2\beta_k\left[A(k)^\dagger - A(k)\right]\right\} \qquad \text{(C1)}$$

and

$$|n(k)\rangle = \frac{1}{\sqrt{n(k)}}A(k)^{\dagger n(k)}|0\rangle \qquad \text{(C2)}$$

respectively. Here $|0\rangle$ is the vacuum state of the resoator array, $A(k)^\dagger$ is defined in Eq. (6). We further define the function $f(\vec{\beta})$ as

$$f(\vec{\beta}) = \prod_k \langle n(k)|\mathcal{U}_k[\beta_k]|n'(k)\rangle \qquad \text{(C3)}$$

with

$$\vec{\beta} = (\beta_{k_1}, \beta_{k_2}, ...). \qquad \text{(C4)}$$

The straightforward calculation shows that

$$
\begin{aligned}
f(\vec{\beta}) &= \prod_k \langle n(k)|\mathcal{U}_k[\beta_k]|n'(k)\rangle \\
&= \prod_k e^{-|2\beta_k|^2/2}\langle n(k)|e^{-2\beta_k A(k)^\dagger}e^{2\beta_k A(k)}|n'(k)\rangle \\
&= \prod_k \left(e^{-|2\beta_k|^2/2} \sum_{m=\text{Max}[0,n'(k)-n(k)]}^{n'(k)} \frac{[2\beta(k)]^m [-2\beta_k]^{n(k)-n'(k)+m}}{m![n(k)-n'(k)+m]!}\langle n(k)|A(k)^{\dagger m}A(k)^m|n'(k)\rangle \right),
\end{aligned}
$$

$$\text{(C5)}$$

which gives

$$f(-\vec{\beta}) = (-1)^{N(\vec{n})-N(\vec{n}')}f(\vec{\beta}) \qquad \text{(C6)}$$

or

$$f(-\vec{\beta}) = f(\vec{\beta}) \qquad \text{for} \quad N(\vec{n}) = N(\vec{n}'). \qquad \text{(C7)}$$

On the other hand, with the above definitions and straightforward calculations, we have

$$\langle +,\vec{n}|-,\vec{n}'\rangle = f(\vec{\beta}_0); \qquad \text{(C8)}$$
$$\langle -,\vec{n}|+,\vec{n}'\rangle = f(-\vec{\beta}_0), \qquad \text{(C9)}$$

where $|\pm,\vec{n}\rangle$ are the eigen-states of the Hamiltonian H_1 defined in Sec. IIB and $\vec{\beta}_0 = (\beta_{0k_1}, \beta_{0k_2}, ...)$. Here we have

$$\beta_{0k} = \frac{1}{\sqrt{2\pi}}\sum_{l=-\infty}^{+\infty}\alpha_l e^{ikl} \qquad \text{(C10)}$$

with α_l defined in Eq. (10). Then using Eq. (14) and Eq. (17), we re-write the matrix element $H_{\vec{n}',-}^{\vec{n},+}$ as

$$
\begin{aligned}
H_{\vec{n}',-}^{\vec{n},+} &= \langle \Psi_{+,\vec{n}}|H|\Psi_{+,\vec{n}}\rangle \\
&= \langle \Psi_{+,\vec{n}}|H_2|\Psi_{-,\vec{n}'}\rangle \\
&= \frac{\Omega}{4}(\langle +,\vec{n}|-,\vec{n}'\rangle - \langle -,\vec{n}|+,\vec{n}'\rangle) \\
&= \frac{\Omega}{4}\left[f(\vec{\beta}_0) - f(-\vec{\beta}_0)\right] \qquad \text{(C11)}
\end{aligned}
$$

Therefore, our above result in Eq. (C7) directly leads to Eq. (19).

Appendix D: The unitary operator U_M

In this appendix, we calculate the unitary operator U_M defined in (48). Similar as in appendix B, it is easy to prove that U_{TM} is the product of the displacement operators of each resonator mode:

$$U_M = \prod_{j=-\infty}^{+\infty}\exp[\alpha_j^M\sigma_x(a_j^\dagger - a_j)]. \qquad \text{(D1)}$$

To derive the expression of α_j^M, we define the column vector

$$\vec{\alpha} = \left(...\alpha_{-1}^M, \alpha_0^M, \alpha_1^M, ...\right)^T. \qquad \text{(D2)}$$

Then the straightforward calculation shows that, the condition (48) is equivalent to the equation

$$\omega\vec{\alpha} - \xi K\vec{\alpha} = \vec{\Lambda}. \qquad \text{(D3)}$$

Here K is a square matrix with the element K_{ij} in the i-th row and j-th column given by

$$K_{ij} = \delta_{i,j+1} + \delta_{i,j-1} \qquad \text{(D4)}$$

In Eq. (D3), $\vec{\Lambda}$ is a constant column vector with the j-th component Λ_j defined as

$$\Lambda_j = \lambda\sum_{\beta=1}^{m}\delta_{j,c(\beta)}. \qquad \text{(D5)}$$

Therefore, we formally have the expression of $\vec{\alpha}$:

$$\vec{\alpha} = \frac{1}{\omega - \xi K}\vec{\Lambda}. \tag{D6}$$

Furthermore, we notice that the matrix $\omega - \xi K$ is diagonalized as

$$\omega - \xi K = \int dk\, (\omega - 2\xi \cos k)\, \vec{v}(k)\vec{v}(k)^{\dagger} \tag{D7}$$

with the j-th component of the column vector $\vec{v}(k)$ satisfies

$$v_j(k) = \frac{1}{\sqrt{2\pi}}e^{ikj}. \tag{D8}$$

Then we have

$$\frac{1}{\omega - \xi K} = \int dk \frac{\vec{v}(k)\vec{v}(k)^{\dagger}}{\omega - 2\xi \cos k}. \tag{D9}$$

Substituting (D9) into (D6), we get the expression of α_j^M:

$$\alpha_j^M = \frac{\lambda}{2\pi} \sum_{\beta=1}^{m} \int dk \frac{\exp\left[ik\left(j - c\left(\beta\right)\right)\right]}{\omega - 2\xi \cos k}. \tag{D10}$$

In the case of a single TLS located the 0-th resonator, we have $m = 1$ and $c\,(1) = 0$. Then α_j^M is expressed as

$$\alpha_j^M = \frac{\lambda}{2\pi} \int dk \frac{\exp\left[ikj\right]}{\omega - 2\xi \cos k}. \tag{D11}$$

On the other hand, in such a single-TLS case, the value of α_j^M is also given by (B11). Therefore, we have

$$\frac{\lambda}{2\pi} \int dk \frac{\exp\left[ikj\right]}{\omega - 2\xi \cos k} = \frac{\lambda\omega_1}{2\xi^2 - \omega\omega_1}(\frac{\xi}{\omega_1})^{|j|} \tag{D12}$$

with ω_1 defined in Sec.II.B. Substituting (D12) into (D10), we finally obtain

$$\alpha_j^M = \sum_{\beta=1}^{m} \frac{\lambda\omega_1}{2\xi^2 - \omega\omega_1}(\frac{\xi}{\omega_1})^{|j-c(\beta)|}. \tag{D13}$$

Therefore, we get the analytical expression of the unitary operator U_M defined in Eqs. (48, D1).

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